Department 1411 Review
May 16, 2006
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Verification & Validation (V&V)	0.50 time
SciDAC (Interoperable Tools)	0.25 time
Meshing Research (Optimization, Accuracy, & Efficiency)	0.25 time

SAND2006-3617P

Measuring Progress in Code Order-Verification

Programmatic Issue: How does one demonstrate progress in V&V? (Kusnezov)

Activities: SAND report “Measuring Progress in Order-Verification”, Premo Demonstration (Ober & Bond)

Thesis: Order-verification is (nearly) a close-ended process.
Can therefore create comprehensive test-suite (OVTS)
and measure progress in testing the code.

$$Fitness = \sum_{n=1}^{N} \sum_{j=1}^{J} w_{n,j} r_{n,j}$$

Results: Creating a comprehensive OVTS was time-consuming and fraught with uncertainty because order-verification was an after-thought in code development, not intrinsic.

I am featured-speaker in USNCCM sessions on V&V.
Two Journal Articles in progress.

Impact: Example for other code dev. groups to follow;
Basis for justifying need for support to do verification.
Help ASC V&V; National Center for Excellence

Verification Software Toolkit (VST)

Programmatic Issue: Provide 'Institutional Solution' to pre- and post-processing needs for order-verification to avoid duplication (re-inventing the wheel) and to encourage the practice of order-verification.

Activities: VST Functional Requirements SAND, Bi-weekly meetings with DSTK group, Interactions with users.

Knupp, 0.10 FTE
Jones, 0.20 FTE
Weirs, 0.10 FTE

Technical: Post-processing FEM Solutions for Order-Verification (Hetmaniuk)

$$\left\| u - u_h \right\| \approx \left\| u_I - u_h \right\| \quad as \quad h \to 0$$

Results: VST post-processing code based on DSTK with real users

Impact: Uniformity of reporting, provides users access to functionalities not developed by themselves, parallel processing via DSTK, VVMethods, VST in ITAPS, VST in HEDP and other IPT's. Lays groundwork for future enhancements and for pre-processing capability.

Coordination of ASC Verification Activities

Programmatic Issue: Coordinate on-going ASC verification activities (Pilch)

Activities:

Exchange of information & knowledge, take advantage of synergies,
Meetings with Alegra (sustainable verification, move from regression-based testing to verification-based);
Calore (Dowding & Blackwell), Fuego (Luketa-Hanlin); Premo (Bond & Ober);
Bova, Charon (Hoekstra & Hennigan)

Technical: L-inf norm is h^2 log(h)

Results: Common knowledge of VST, Progress, each other

Impact: Better work

New Initiatives in V&V

HEDP IPT – Role: contribute ideas, experience, research on code verification within IPT

Contributions to Memo to Algorithms on V&V: Currently, the code is the model of physical reality, not the governing equations; (diminishes the role of algorithms)

National Center for Excellence:

- SNL assume Leadership role for setting National Agenda on V&V
- Pilch: asked me to work on draft based on “levels of maturity” in verification.

24 Open Questions in MMS:

- Key research questions for code order-verification need attention.

Mesh Optimization & R-adaptivity Research

MICS 3-year grant:
"R-adaptive mesh quality improvement using the Target-matrix paradigm"
SNL, ANL, LLNL
(Knupp – quarter-time, Hetmaniuk - half-time)

Research Goals:
- Complete Target-matrix Theory, (4 papers in SISC)
- New numerical optimization algorithms for Mesh Optimization
- Completed study of High-Level Optimization Techniques
- Applications demonstrations: Rezone (Alegra, LLNL); G-adaptivity;
  Deforming Domains (SLAC, Dakota); Post-processing (mesh generators)
- r-adaptive and hr-adaptivity
- Impact of Mesh on Solution Accuracy & Efficiency

Impact: More capable methods for applications; faster methods; a new theory on the significance level of harmonic mappings & Laplace-Beltrami.

New Research Initiative:
Impact of Mesh on Solution Accuracy & Efficiency

Literature Survey (35pp): Hetmaniuk & Knupp (0.125 FTE)

Activity: Survey FEM literature for results on error bounds & mesh quality

Goal: understand what's known & identify gaps

Viewpoint: mesh-oriented (how can one create better meshes using these bounds?)

Broad Scope: For what meshes is discrete maximum principle violated?
Impact on Efficiency (little known)

Impact: R-adaptive Algorithms,
Survey paper in SIAM Review,
CSRI Workshop (fill in gaps)

Summary Table: Impact of Mesh on Solution Accuracy

Case	**Linear Triangle**	**Curved Triangle**
General	Ciarlet, Shewchuk	Ciarlet, Zlamal
Solution-dependent	Apel, Cao, Huang, Formaggia & Perotto	None
PDE-dependent	Bernardi & Verfurth	None
Case	**Parallelogram**	**Convex Quad**
General	Ciarlet	Acosta & Duran, Ciarlet, Jamet, Zenisek
Solution-dependent	Apel, Formaggia & Perotto, Huang	Apel
PDE-dependent	Bernardi & Verfurth	None
Case	**Linear Tetrahedron**	**Curved Tetrahedron**
General	Ciarlet, Shewchuk	Ciarlet
Solution-dependent	Apel, Berzins, Formaggia, Huang	None
PDE-dependent	Bernardi & Verfurth	None
Case	**Parallelepiped**	**Hexahedron**
General	Ciarlet	Ciarlet
Solution-dependent	Apel, Formaggia, Huang	Apel
PDE-dependent	Bernardi & Verfurth	None

Meshing Research: Target Paradigm (measuring quality relative to the application)

I. Knupp, ,"*Formulation of a Target-Matrix Paradigm (TMP) for Mesh Optimization*,"
submitted to SISC

Contents: Mathematical description & analysis of basic objects in paradigm:
Active, Target, Weighted Matrices, Local Metrics, Non-local Metrics, Objective Functions
Significance: Unified approach to mesh optimization that targets all known applications
(list of apps)

II. Knupp, "*Updating Meshes on Deforming Domains within the Target Paradigm*,"
submitted to Communications in Numerical Methods in Engineering,
(Invited paper); USNCCM Austin (presentation)

Knupp
0.125 FTE

Contents: Use of particular TMP local metrics to update meshes on deforming domains
Significance: Design optimization (SLAC, Dakota, ddrv)

III. Knupp, Diachin, Munson, Shontz, "*A Comparison of Two Optimization Methods for Mesh Quality Improvement*," accepted for publication in Engr. with Computers.

Contents: Empirical comparisons of Coordinate Descent vs. Global Optimization
Significance: In-depth study on high-level optimization approaches for speed

IV. Knupp, van der Zee "*Global Convexity of Target-matrix Objective Functions*,"
in progress

Contents: Proofs of Strict Convexity of Target-matrix Objective Functions given local convexity of metrics
Significance: Strict Convexity implies Unique Solutions for Mesh Optimization

SciDAC-I: TSTT

TSTT (Terascale Tools & Technologies) 2001-2006, Knupp (0.25) & Tautges

FY06 TSTT Accomplishments (Knupp, Kraftcheck, Brewer)

Mesquite Website (Knupp)

New Mesquite Customers
- DDRV/Dakota (Tautges)
- SCIRun (Johnson, Shepherd)

Other Major Customers: Alegra HEDP (Grand Challege LDRD: Voth & Brewer), SLAC

Mesquite Architecture Revised to Incorporate full Target-matrix paradigm (Kraftcheck)

SciDAC 2005 (San Francisco), 2006 (Denver) – Invited Poster on Mesquite

Legacy: TSTT, in some small way, blazed the way for current crop of SNL SciDAC proposals by helping to establish SNL as productive SciDAC contributor.

SciDAC-II: ITAPS Proposal

Title: Interoperable Tools for Advanced Petascale Simulations (ITAPS)

Staff: Knupp (PI), Tautges, Devine

ITAPS Enabling Technology Center is TSTT follow-on

Charter: Develop interoperable/interchangeable mesh, geometry, and field manipulation tools for SciDAC applications

Customers: Particle Accelerators, Fusion, **Radiation Transport, Astrophysics**, Groundwater, Biology, Nanophotonics

Products: **Open source geometry tools, deforming geometry, parallel mesh generation, mesh improvement, mesh r-adapt**, mesh h-adapt, front-tracking, error estimation, solution transfer, **dynamic partitioning, code verification**

Budget: Large proposal from SNL (5 labs + 2 universities);
Increase from SNL/TSTT levels

SciDAC SAP:

"Optimal Mesh Generation for Magnetic Fusion Plasma Simulations"
SNL, LLNL, NYU, TechX

Publications

1. Tautges, Knupp, Kraftcheck, and Kim, "Interoperable Geometry and Mesh Components for SciDAC Applications," pp486-490, in SciDAC 2005, A. Mezzecappa ed., Journal of Physics Conference Series, Vol. 16, 2005.

2. Diachin, Knupp, Munson, Shontz, "*A Comparison of Two Optimization Methods for Mesh Quality Improvement*," accepted for publication in Engr. with Computers.

3. Knupp, "Measuring Progress in Code Order-Verification," SAND2005-6894.

4. Knupp, "Functional Requirements for a Verification Software Toolkit," SAND2006-0882P.

5. Knupp, ,"*Formulation of a Target-Matrix Paradigm (TMP) for Mesh Optimization*," submitted to SISC

6. Knupp, "*Updating Meshes on Deforming Domains within the Target Paradigm*," invited submission to Communications in Numerical Methods in Engineering,